Tetraethylenepentamine
112-57-2 | DTXSID7026108

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 52.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 2.80e-01

Confidence level: 4.86e-01

Nearest Neighbors from the Training Set

Image not found
Cymoxanil
Measured: 123
Predicted: 72.0

Image not found
Monocrotophos
Measured: 1.00
Predicted: 2.76

Image not found
Phenazopyridine
Measured: 209
Predicted: 268

Image not found
Glufosinate-ammonium
Measured: 427
Predicted: 194

Image not found
Asulam
Measured: 39.8
Predicted: 38.8